



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:55 PM UTC

PDB ID : 3WOM / pdb_00003wom
Title : Crystal structure of the DAP BII dipeptide complex II
Authors : Sakamoto, Y.; Suzuki, Y.; Iizuka, I.; Tateoka, C.; Roppongi, S.; Fujimoto, M.;
Nonaka, T.; Ogasawara, W.; Tanaka, N.
Deposited on : 2013-12-29
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

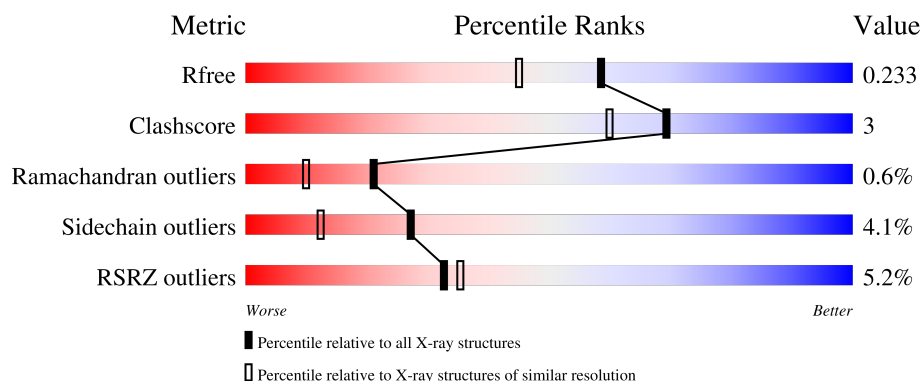
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	698	 90% 9% .
1	B	698	 10% 85% 13% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	804	-	-	X	-

2 Entry composition [i](#)

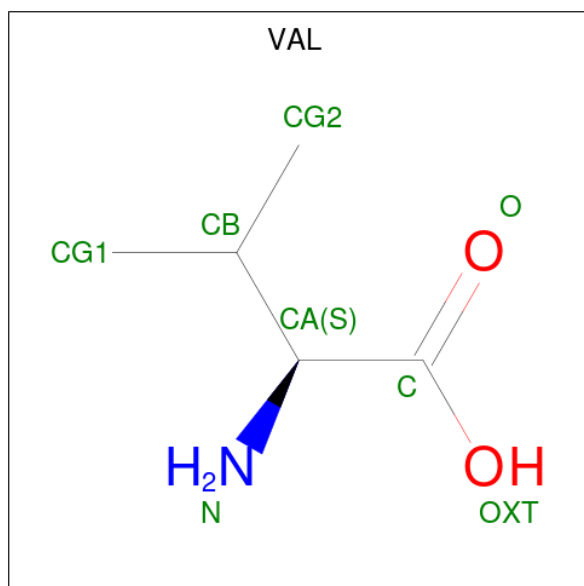
There are 6 unique types of molecules in this entry. The entry contains 11830 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called dipeptidyl aminopeptidase BII.

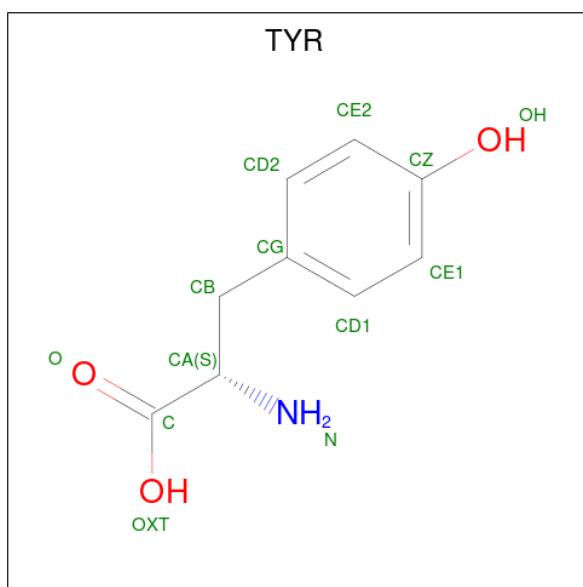
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	697	Total	C	N	O	S	0	0	0
			5371	3398	937	1017	19			
1	B	697	Total	C	N	O	S	0	0	0
			5371	3398	937	1017	19			

- Molecule 2 is VALINE (CCD ID: VAL) (formula: $C_5H_{11}NO_2$).



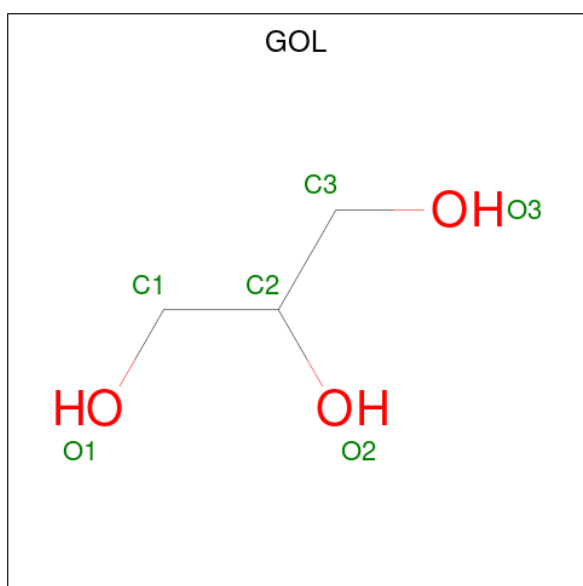
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is TYROSINE (CCD ID: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		
3	B	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		

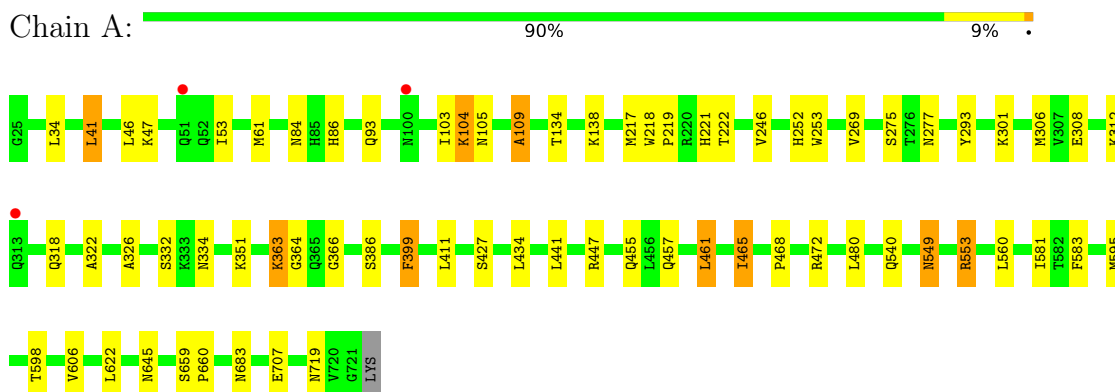
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	584	Total	O	0	0
			584	584		
6	B	400	Total	O	0	0
			400	400		

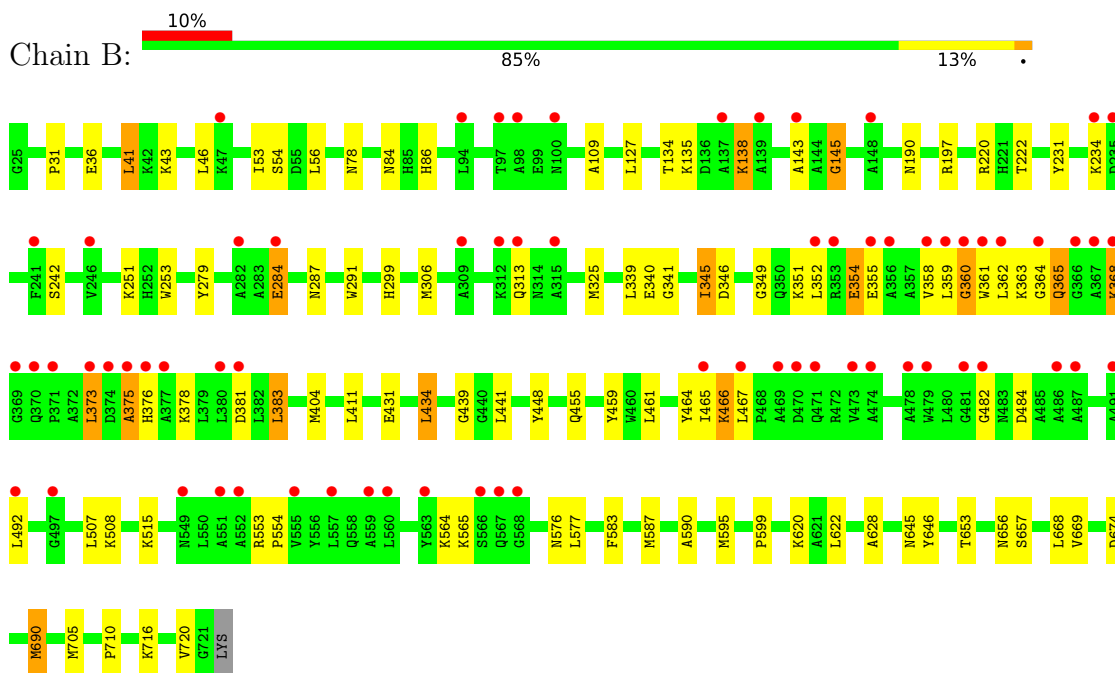
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: dipeptidyl aminopeptidase BII



• Molecule 1: dipeptidyl aminopeptidase BII



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	122.22Å 122.22Å 219.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.21 – 1.86 39.21 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.21-1.86) 98.3 (39.21-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.183 , 0.225 0.192 , 0.233	Depositor DCC
R_{free} test set	6897 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11830	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1937e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.29	9/5489 (0.2%)	1.13	10/7440 (0.1%)
1	B	1.19	2/5489 (0.0%)	1.12	16/7440 (0.2%)
All	All	1.24	11/10978 (0.1%)	1.13	26/14880 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	6
All	All	0	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	TRP	CA-C	7.71	1.59	1.52
1	A	326	ALA	N-CA	6.08	1.53	1.46
1	A	457	GLN	N-CA	5.93	1.53	1.46
1	A	334	ASN	CG-ND2	-5.90	1.20	1.33
1	A	246	VAL	CA-C	5.62	1.57	1.52
1	A	217	MET	N-CA	5.57	1.52	1.45
1	A	660	PRO	C-O	5.53	1.29	1.23
1	B	668	LEU	CA-C	5.46	1.60	1.52
1	A	322	ALA	C-O	-5.32	1.17	1.24
1	A	332	SER	N-CA	-5.12	1.40	1.46
1	A	399	PHE	C-O	-5.08	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	LYS	N-CA-C	-6.67	104.08	111.36
1	B	325	MET	CG-SD-CE	-6.04	87.60	100.90
1	B	284	GLU	CB-CG-CD	5.91	122.64	112.60
1	B	345	ILE	CB-CA-C	-5.91	104.35	111.85
1	A	109	ALA	CA-C-N	-5.88	113.62	119.56
1	A	109	ALA	C-N-CA	-5.88	113.62	119.56
1	B	109	ALA	CA-C-N	-5.83	113.67	119.56
1	B	109	ALA	C-N-CA	-5.83	113.67	119.56
1	B	439	GLY	N-CA-C	5.83	119.69	112.64
1	A	553	ARG	CB-CG-CD	5.81	124.67	111.30
1	B	340	GLU	N-CA-C	5.79	118.05	111.11
1	B	78	ASN	N-CA-C	5.74	119.06	112.57
1	B	674	ASP	CA-C-N	5.60	126.04	122.18
1	B	674	ASP	C-N-CA	5.60	126.04	122.18
1	A	598	THR	CA-C-N	-5.58	113.92	119.56
1	A	598	THR	C-N-CA	-5.58	113.92	119.56
1	A	301	LYS	N-CA-C	5.46	117.24	111.28
1	B	628	ALA	N-CA-C	5.45	119.79	113.20
1	B	284	GLU	N-CA-C	-5.33	105.37	111.07
1	A	103	ILE	N-CA-C	-5.31	105.32	110.42
1	B	669	VAL	N-CA-C	5.25	117.94	112.90
1	B	351	LYS	N-CA-C	-5.20	104.53	111.24
1	A	293	TYR	CA-C-N	-5.18	113.30	119.05
1	A	293	TYR	C-N-CA	-5.18	113.30	119.05
1	B	587	MET	CA-C-N	-5.00	117.05	122.55
1	B	587	MET	C-N-CA	-5.00	117.05	122.55

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	LYS	Peptide
1	B	145	GLY	Peptide
1	B	313	GLN	Peptide
1	B	363	LYS	Peptide
1	B	465	ILE	Peptide
1	B	482	GLY	Peptide
1	B	720	VAL	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5371	0	5284	32	0
1	B	5371	0	5284	42	0
2	A	7	0	8	0	0
2	B	7	0	8	0	0
3	A	13	0	9	0	0
3	B	13	0	9	1	0
4	A	36	0	48	8	0
4	B	24	0	32	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	584	0	0	6	0
6	B	400	0	0	2	0
All	All	11830	0	10682	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (75) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLU:O	1:B:358:VAL:HG23	1.72	0.88
1:A:252:HIS:HD1	4:A:804:GOL:HO1	1.12	0.88
4:A:806:GOL:H11	6:A:1101:HOH:O	1.75	0.86
1:A:549:ASN:ND2	6:A:1478:HOH:O	2.17	0.77
1:A:252:HIS:ND1	4:A:804:GOL:O1	2.11	0.75
1:B:346:ASP:OD2	1:B:349:GLY:HA3	1.92	0.68
1:A:109:ALA:O	6:A:1260:HOH:O	2.13	0.65
1:B:299:HIS:HD2	1:B:459:TYR:OH	1.80	0.64
1:B:362:LEU:HA	1:B:365:GLN:OE1	1.98	0.64
1:B:36:GLU:OE1	6:B:1256:HOH:O	2.14	0.64
4:A:806:GOL:C1	6:A:1101:HOH:O	2.42	0.62
1:A:549:ASN:HD21	1:A:553:ARG:HE	1.48	0.61
1:A:707:GLU:OE2	6:A:1438:HOH:O	2.16	0.59
1:A:595:MET:HE3	1:B:595:MET:CE	2.33	0.58
1:A:252:HIS:CE1	4:A:804:GOL:HO1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MET:HE1	1:A:581:ILE:HD11	1.86	0.58
1:B:431:GLU:HA	1:B:434:LEU:HD22	1.87	0.57
1:B:41:LEU:HG	1:B:46:LEU:HD22	1.89	0.55
1:B:411:LEU:HD21	1:B:441:LEU:HD11	1.89	0.54
1:B:253:TRP:CE2	4:B:804:GOL:H32	2.43	0.54
1:A:134:THR:HG22	1:A:138:LYS:HD2	1.90	0.53
1:A:93:GLN:NE2	1:A:447:ARG:HE	2.07	0.53
1:B:365:GLN:O	1:B:368:LYS:HE3	2.09	0.53
1:B:590:ALA:O	1:B:690:MET:HE1	2.08	0.53
1:B:653:THR:H	1:B:656:ASN:HD22	1.57	0.52
1:A:222:THR:H	1:A:645:ASN:HD21	1.58	0.52
1:B:134:THR:HG22	1:B:138:LYS:HD3	1.90	0.52
1:A:411:LEU:HD21	1:A:441:LEU:HD11	1.92	0.52
1:A:104:LYS:HD3	1:A:105:ASN:OD1	2.10	0.52
4:A:808:GOL:H32	6:A:1441:HOH:O	2.10	0.52
1:B:484:ASP:N	1:B:484:ASP:OD1	2.44	0.50
1:A:622:LEU:C	1:A:622:LEU:HD23	2.37	0.50
1:B:222:THR:H	1:B:645:ASN:HD21	1.61	0.49
1:B:53:ILE:O	1:B:53:ILE:HG22	2.13	0.49
1:B:306:MET:CE	1:B:455:GLN:HB3	2.43	0.49
1:A:84:ASN:HD22	1:A:86:HIS:CE1	2.30	0.48
1:A:465:ILE:HD11	1:A:480:LEU:HD21	1.94	0.48
1:B:576:ASN:O	1:B:577:LEU:HB2	2.13	0.48
1:B:373:LEU:HD23	1:B:373:LEU:O	2.14	0.48
1:A:306:MET:HE3	1:A:455:GLN:HB3	1.97	0.47
1:A:277:ASN:HD22	1:A:683:ASN:HD21	1.63	0.47
1:B:31:PRO:HB3	1:B:56:LEU:HD21	1.98	0.46
1:B:41:LEU:HD13	1:B:583:PHE:CG	2.50	0.46
1:A:41:LEU:HD13	1:A:583:PHE:CG	2.51	0.46
1:B:622:LEU:C	1:B:622:LEU:HD23	2.42	0.45
1:B:220:ARG:HB3	1:B:645:ASN:HD22	1.81	0.45
1:B:145:GLY:HA2	6:B:1244:HOH:O	2.18	0.44
1:B:127:LEU:HA	1:B:190:ASN:HD22	1.81	0.44
1:B:705:MET:O	1:B:710:PRO:HA	2.17	0.44
1:B:341:GLY:O	1:B:345:ILE:HG12	2.18	0.44
1:B:197:ARG:HD2	1:B:231:TYR:CE1	2.52	0.44
1:A:93:GLN:HE22	1:A:447:ARG:HE	1.66	0.44
1:B:279:TYR:CZ	1:B:564:LYS:HE3	2.53	0.43
1:A:318:GLN:HE21	4:A:807:GOL:H12	1.83	0.43
1:B:84:ASN:HD22	1:B:86:HIS:CE1	2.35	0.43
1:A:595:MET:HE3	1:B:595:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HG	1:A:46:LEU:HD22	2.00	0.42
1:B:284:GLU:HG3	1:B:383:LEU:CD2	2.49	0.42
1:B:359:LEU:O	1:B:360:GLY:C	2.62	0.42
1:A:253:TRP:CE2	4:A:804:GOL:H32	2.54	0.42
1:B:553:ARG:N	1:B:554:PRO:CD	2.82	0.41
1:B:599:PRO:O	1:B:646:TYR:HA	2.21	0.41
1:A:47:LYS:HD3	1:A:47:LYS:HA	1.88	0.41
1:B:464:TYR:CD1	1:B:467:LEU:HD12	2.55	0.41
1:B:404:MET:HE3	1:B:448:TYR:CE1	2.56	0.41
1:B:657:SER:OG	3:B:802:TYR:C	2.64	0.41
1:A:269:VAL:HG13	1:A:659:SER:HB3	2.02	0.41
1:A:53:ILE:O	1:A:53:ILE:HG22	2.20	0.41
1:A:218:TRP:CG	1:A:219:PRO:HA	2.56	0.41
1:B:383:LEU:HD12	1:B:383:LEU:O	2.21	0.41
1:A:221:HIS:HB3	1:A:606:VAL:HG22	2.04	0.40
1:A:399:PHE:CZ	1:A:461:LEU:HD13	2.56	0.40
1:B:375:ALA:O	1:B:376:HIS:C	2.63	0.40
1:A:468:PRO:O	1:A:472:ARG:HG2	2.21	0.40
1:B:361:TRP:O	1:B:365:GLN:OE1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	695/698 (100%)	678 (98%)	14 (2%)	3 (0%)	30	17
1	B	695/698 (100%)	660 (95%)	30 (4%)	5 (1%)	18	8
All	All	1390/1396 (100%)	1338 (96%)	44 (3%)	8 (1%)	21	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	364	GLY
1	B	466	LYS
1	A	364	GLY
1	A	366	GLY
1	B	143	ALA
1	A	719	ASN
1	B	375	ALA
1	B	360	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	541/542 (100%)	526 (97%)	15 (3%)	38	23
1	B	541/542 (100%)	511 (94%)	30 (6%)	19	6
All	All	1082/1084 (100%)	1037 (96%)	45 (4%)	27	12

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	41	LEU
1	A	104	LYS
1	A	275	SER
1	A	308	GLU
1	A	312	LYS
1	A	363	LYS
1	A	386	SER
1	A	427	SER
1	A	434	LEU
1	A	461	LEU
1	A	465	ILE
1	A	540	GLN
1	A	549	ASN
1	A	560	LEU
1	B	41	LEU

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Mol	Chain	Res	Type
1	B	43	LYS
1	B	54	SER
1	B	135	LYS
1	B	138	LYS
1	B	234	LYS
1	B	242	SER
1	B	251	LYS
1	B	287	ASN
1	B	339	LEU
1	B	352	LEU
1	B	354	GLU
1	B	355	GLU
1	B	365	GLN
1	B	368	LYS
1	B	373	LEU
1	B	378	LYS
1	B	381	ASP
1	B	383	LEU
1	B	434	LEU
1	B	461	LEU
1	B	466	LYS
1	B	492	LEU
1	B	507	LEU
1	B	508	LYS
1	B	515	LYS
1	B	565	LYS
1	B	620	LYS
1	B	690	MET
1	B	716	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	93	GLN
1	A	277	ASN
1	A	303	GLN
1	A	318	GLN
1	A	385	GLN
1	A	400	ASN
1	A	471	GLN
1	A	521	ASN

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Mol	Chain	Res	Type
1	A	540	GLN
1	A	549	ASN
1	A	585	ASN
1	A	645	ASN
1	A	656	ASN
1	B	84	ASN
1	B	93	GLN
1	B	190	ASN
1	B	277	ASN
1	B	299	HIS
1	B	303	GLN
1	B	318	GLN
1	B	365	GLN
1	B	376	HIS
1	B	585	ASN
1	B	645	ASN
1	B	656	ASN
1	B	719	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	TYR	B	802	2	12,13,13	1.25	1 (8%)	13,17,17	0.92	0
4	GOL	A	808	-	5,5,5	0.41	0	5,5,5	0.72	0
4	GOL	A	806	-	5,5,5	0.62	0	5,5,5	1.37	1 (20%)
4	GOL	B	803	-	5,5,5	0.44	0	5,5,5	0.69	0
4	GOL	B	804	-	5,5,5	0.84	0	5,5,5	0.94	0
4	GOL	A	803	-	5,5,5	0.13	0	5,5,5	0.81	0
4	GOL	A	805	-	5,5,5	0.67	0	5,5,5	0.39	0
4	GOL	B	805	-	5,5,5	0.56	0	5,5,5	0.52	0
2	VAL	A	801	3	4,6,7	0.80	0	6,7,9	0.51	0
4	GOL	B	806	-	5,5,5	0.68	0	5,5,5	1.19	0
4	GOL	A	804	-	5,5,5	0.39	0	5,5,5	2.31	1 (20%)
3	TYR	A	802	2	12,13,13	1.63	5 (41%)	13,17,17	1.11	1 (7%)
2	VAL	B	801	3	4,6,7	0.64	0	6,7,9	1.05	1 (16%)
4	GOL	A	807	-	5,5,5	0.40	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYR	B	802	2	-	6/8/8/8	0/1/1/1
4	GOL	A	808	-	-	3/4/4/4	-
4	GOL	A	806	-	-	4/4/4/4	-
4	GOL	B	803	-	-	0/4/4/4	-
4	GOL	B	804	-	-	2/4/4/4	-
4	GOL	A	803	-	-	0/4/4/4	-
4	GOL	A	805	-	-	1/4/4/4	-
4	GOL	B	805	-	-	1/4/4/4	-
2	VAL	A	801	3	-	0/5/6/8	-
4	GOL	B	806	-	-	1/4/4/4	-
4	GOL	A	804	-	-	0/4/4/4	-
3	TYR	A	802	2	-	4/8/8/8	0/1/1/1
2	VAL	B	801	3	-	1/5/6/8	-
4	GOL	A	807	-	-	1/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	TYR	CE2-CZ	-2.56	1.34	1.39
3	A	802	TYR	OXT-C	-2.48	1.22	1.30
3	B	802	TYR	CE2-CZ	-2.37	1.34	1.39
3	A	802	TYR	CE1-CD1	2.16	1.42	1.38
3	A	802	TYR	OH-CZ	2.08	1.41	1.37
3	A	802	TYR	CD2-CG	2.06	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	804	GOL	O1-C1-C2	-4.68	89.30	110.38
3	A	802	TYR	OXT-C-O	-2.48	118.45	124.08
2	B	801	VAL	CB-CA-C	-2.14	109.95	112.87
4	A	806	GOL	O3-C3-C2	2.08	119.76	110.38

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	GOL	O1-C1-C2-C3
4	A	808	GOL	C1-C2-C3-O3
4	B	804	GOL	O1-C1-C2-C3
4	A	806	GOL	C1-C2-C3-O3
4	A	806	GOL	O1-C1-C2-O2
4	A	808	GOL	O2-C2-C3-O3
4	A	806	GOL	O2-C2-C3-O3
4	B	804	GOL	O1-C1-C2-O2
4	A	805	GOL	O2-C2-C3-O3
4	B	805	GOL	O1-C1-C2-O2
3	B	802	TYR	OXT-C-CA-CB
3	A	802	TYR	O-C-CA-CB
4	A	808	GOL	O1-C1-C2-C3
3	A	802	TYR	OXT-C-CA-CB
2	B	801	VAL	C-CA-CB-CG1
3	A	802	TYR	CA-CB-CG-CD1
4	A	807	GOL	O1-C1-C2-O2
4	B	806	GOL	O1-C1-C2-O2
3	B	802	TYR	O-C-CA-CB
3	A	802	TYR	CA-CB-CG-CD2
3	B	802	TYR	C-CA-CB-CG
3	B	802	TYR	CA-CB-CG-CD2
3	B	802	TYR	CA-CB-CG-CD1
3	B	802	TYR	O-C-CA-N

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	TYR	1	0
4	A	808	GOL	1	0
4	A	806	GOL	2	0
4	B	804	GOL	1	0
4	A	804	GOL	4	0
4	A	807	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	697/698 (99%)	-0.25	3 (0%) 88 91	9, 22, 36, 54	0
1	B	697/698 (99%)	0.52	69 (9%) 13 12	12, 31, 54, 83	0
All	All	1394/1396 (99%)	0.14	72 (5%) 33 35	9, 25, 49, 83	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	469	ALA	5.0
1	B	373	LEU	4.8
1	B	478	ALA	4.4
1	B	361	TRP	4.2
1	B	549	ASN	4.0
1	B	352	LEU	3.7
1	B	309	ALA	3.7
1	B	366	GLY	3.5
1	B	481	GLY	3.4
1	B	246	VAL	3.3
1	B	368	LYS	3.3
1	B	467	LEU	3.2
1	B	492	LEU	3.2
1	A	51	GLN	3.2
1	B	369	GLY	3.2
1	B	555	VAL	3.1
1	B	482	GLY	3.1
1	B	374	ASP	3.1
1	B	377	ALA	3.1
1	B	364	GLY	3.0
1	B	474	ALA	3.0
1	B	358	VAL	2.9
1	B	381	ASP	2.9
1	B	486	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	376	HIS	2.9
1	B	359	LEU	2.9
1	B	497	GLY	2.8
1	B	557	LEU	2.8
1	B	380	LEU	2.8
1	B	375	ALA	2.7
1	B	551	ALA	2.7
1	B	371	PRO	2.7
1	B	563	TYR	2.6
1	B	356	ALA	2.6
1	B	362	LEU	2.6
1	B	470	ASP	2.6
1	B	148	ALA	2.6
1	B	360	GLY	2.5
1	B	315	ALA	2.5
1	B	473	VAL	2.5
1	B	479	TRP	2.5
1	B	312	LYS	2.5
1	B	100	ASN	2.4
1	B	234	LYS	2.4
1	B	568	GLY	2.3
1	B	313	GLN	2.3
1	B	353	ARG	2.3
1	B	97	THR	2.3
1	B	98	ALA	2.3
1	B	139	ALA	2.3
1	B	487	ALA	2.3
1	B	491	ALA	2.3
1	B	552	ALA	2.3
1	A	100	ASN	2.3
1	B	355	GLU	2.2
1	B	367	ALA	2.2
1	B	47	LYS	2.2
1	B	560	LEU	2.2
1	B	559	ALA	2.2
1	B	370	GLN	2.2
1	B	471	GLN	2.2
1	B	567	GLN	2.2
1	B	241	PHE	2.1
1	B	235	ASP	2.1
1	B	465	ILE	2.1
1	B	566	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLN	2.1
1	B	94	LEU	2.1
1	B	284	GLU	2.0
1	B	137	ALA	2.0
1	B	143	ALA	2.0
1	B	282	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	805	6/6	0.81	0.17	44,51,52,56	0
4	GOL	A	807	6/6	0.82	0.17	36,54,58,62	0
4	GOL	B	804	6/6	0.86	0.16	36,44,50,53	0
4	GOL	A	805	6/6	0.90	0.12	36,40,42,42	0
4	GOL	A	806	6/6	0.91	0.12	34,44,47,50	0
4	GOL	A	804	6/6	0.93	0.10	29,34,36,38	0
4	GOL	B	806	6/6	0.93	0.09	24,34,36,38	0
4	GOL	A	808	6/6	0.94	0.10	20,33,40,46	0
5	ZN	A	810	1/1	0.94	0.21	54,54,54,54	0
3	TYR	B	802	13/13	0.96	0.06	17,20,25,28	0
3	TYR	A	802	13/13	0.96	0.06	12,16,20,26	0
2	VAL	B	801	7/8	0.97	0.05	14,14,15,17	0
4	GOL	B	803	6/6	0.97	0.05	16,17,21,22	0
4	GOL	A	803	6/6	0.97	0.05	15,16,18,19	0
5	ZN	B	807	1/1	0.97	0.06	32,32,32,32	0
5	ZN	B	808	1/1	0.97	0.20	49,49,49,49	0
2	VAL	A	801	7/8	0.98	0.05	10,12,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	A	809	1/1	0.99	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.